Renormalization of the electron–phonon interaction: a reformulation of the BCS–gap equation

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A recently developed renormalization approach is used to study the electron-phonon coupling in many-electron systems. By starting from an Hamiltonian which includes a small gauge symmetry breaking field, we directly derive a BCS-like equation for the energy gap from the renormalization approach. The effective electron-electron interaction for Cooper pairs does not contain any singularities. Furthermore, it is found that phonon-induced particle-hole excitations only contribute to the attractive electron-electron interaction if their energy difference is smaller than the phonon energy.

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I. INTRODUCTION

The famous BCS-theory [1] of superconductivity is essentially based on the analysis of attractive interactions between electrons of many-particle systems [2]. As was pointed out by Fröhlich [3] such an interaction can result from an effective coupling between electrons mediated via phonons. The recent discovery of superconductivity in magnesium diboride MgB_2 [4] below a rather high T_c of about 39 K has attracted again a lot of interest on this classical scenario of a phonon-mediated superconductivity. However, the electron-electron interaction derived by Fröhlich [3] contains some problems. There are certain regions in momentum space where the attractive interaction becomes singular and changes its sign due to a vanishing energy denominator.

Recently, effective phonon-induced electron-electron interactions were also derived [5,6] by use of Wegner's flow equation method [7] and by a similarity renormalization proposed by Glatzek and Wilson [8,9]. The main idea of these approaches is to perform a continuous unitary transformation which leads to an expression for an effective electron-electron interaction which is less singular than Fröhlich's result [3].

Recently, we have developed a renormalization approach which is based on perturbation theory [10]. This approach resembles Wegner's flow equation method [7] and the similarity renormalization [8,9] in some aspects. Therefore, the investigation of an effective phonon-induced electron-electron interaction is very useful to compare the three methods in more details. Therefore, in this paper we directly diagonalize the classical problem of interacting electrons and phonons by use of the new renormalization technique [10]. the Hamiltonian is given by

$$\mathcal{H}=\sum_{\mathbf{k},\sigma}\varepsilon_{\mathbf{k}}\,c_{\mathbf{k},\sigma}^{\dagger}c_{\mathbf{k},\sigma}+\sum_{\mathbf{q}}\omega_{\mathbf{q}}\,b_{\mathbf{q}}^{\dagger}b_{\mathbf{q}}+\sum_{\mathbf{k},\mathbf{q},\sigma}\left(g_{\mathbf{q}}\,c_{\mathbf{k},\sigma}^{\dagger}c_{(\mathbf{k}+\mathbf{q}),\sigma}b_{\mathbf{q}}^{\dagger}+g_{\mathbf{q}}^{*}\,c_{(\mathbf{k}+\mathbf{q}),\sigma}^{\dagger}c_{\mathbf{k},\sigma}b_{\mathbf{q}}\right),\tag{1}$$

which will be used to describe superconducting properties. In (1) $c_{\mathbf{k},\sigma}^{\dagger}$ and $c_{\mathbf{k},\sigma}$ are the usual creation and annihilation operators for electrons with wave vector $\mathbf{k}$ and spin σ. $b_{\mathbf{q}}^{\dagger}$ and $b_{\mathbf{q}}$ denote phonon operators with phonon energies $\omega_{\mathbf{q}}$. The electron excitation energies $\varepsilon_{\mathbf{k}}$ are measured from the chemical potential μ.

The paper is organized as follows. In the next section we briefly repeat our recently developed renormalization approach [10]. In Sec. III this approach will be applied to the electron-phonon system (1) in order to derive a BCS-like gap equation. Furthermore, effective electron-electron interaction derived in this framework will be compared with the results from former approaches [3,5,6]. Finally, our conclusions are presented in Sec. IV.

II. PROJECTOR-BASED RENORMALIZATION METHOD (PRM)

The PRM [10] starts from the decomposition of a given many-particle Hamiltonian $\mathcal{H}$ into an unperturbed part $\mathcal{H}_0$ and into a perturbation $\mathcal{H}_1$

$$\mathcal{H}=\mathcal{H}_0+\varepsilon\mathcal{H}_1=:H(\varepsilon).\tag{2}$$

We assume that the eigenvalue problem $\mathcal{H}_0|n\rangle=E_n^{(0)}|n\rangle$ of the unperturbed part $\mathcal{H}_0$ is known. The parameter ε accounts for the order of perturbation processes discussed below. Let us define projection operators $\mathbf{P}_\lambda$ and $\mathbf{Q}_\lambda$ by

$$\mathbf{P}_\lambda A = \sum_{|E_n^{(0)} - E_m^{(0)}| \le \lambda} |n\rangle\langle m| \, \langle n|A|m\rangle \qquad \text{and} \tag{3}$$

$$\mathbf{Q}_\lambda = \mathbf{1} - \mathbf{P}_\lambda. \tag{4}$$

$\mathbf{P}_\lambda$ and $\mathbf{Q}_\lambda$ are super-operators acting on usual operators A of the unitary space. Here, $\mathbf{P}_\lambda$ projects on that part of A which is formed by all transition operators $|n\rangle\langle m|$ with energy differences $|E_n^{(0)} - E_m^{(0)}|$ less or equal to a given cutoff λ. The cutoff λ is smaller than the cutoff Λ of the original Hamiltonian $\mathcal{H}$. $\mathbf{Q}_\lambda$ is orthogonal to $\mathbf{P}_\lambda$ and projects on high energy transitions larger than λ.

The aim is to transform the initial Hamiltonian $\mathcal{H}$ into an effective Hamiltonian $\mathcal{H}_\lambda$ which has no matrix elements between eigenstates of $\mathcal{H}_0$ with energy differences larger than λ. $\mathcal{H}_\lambda$ will be constructed by use of an unitary transformation

$$\mathcal{H}_\lambda = e^{X_\lambda} \, \mathcal{H} \, e^{-X_\lambda}. \tag{5}$$

Due to construction the effective Hamiltonian $\mathcal{H}_\lambda$ will therefore have the same eigenspectrum as the original Hamiltonian $\mathcal{H}$. The generator X_λ of the transformation is anti-Hermitian, $X_\lambda^\dagger = -X_\lambda$. To find an appropriate generator X_λ we use the condition that $\mathcal{H}_\lambda$ has no matrix elements with transition energies larger than λ, i.e.,

$$\mathbf{Q}_\lambda \mathcal{H}_\lambda = 0 \tag{6}$$

has to be fulfilled. By assuming that X_λ can be written as a power series in the perturbation parameter ε

$$X_\lambda = \varepsilon X_\lambda^{(1)} + \varepsilon^2 X_\lambda^{(2)} + \varepsilon^3 X_\lambda^{(3)} + \dots \tag{7}$$

the effective Hamiltonian $\mathcal{H}_\lambda$ can be expanded in a power series in ε as well

$$\begin{aligned} \mathcal{H}_\lambda = \mathcal{H}_0 + \varepsilon \left\{ \mathcal{H}_1 + \left[X_\lambda^{(1)}, \mathcal{H}_0 \right] \right\} + \\ + \varepsilon^2 \left\{ \left[X_\lambda^{(1)}, \mathcal{H}_1 \right] + \left[X_\lambda^{(2)}, \mathcal{H}_0 \right] + \frac{1}{2!} \left[X_\lambda^{(1)}, \left[X_\lambda^{(1)}, \mathcal{H}_0 \right] \right] \right\} + \mathcal{O}(\varepsilon^3). \end{aligned} \tag{8}$$

Now, the high-energy parts parts $\mathbf{Q}_\lambda X_\lambda^{(n)}$ of $X_\lambda^{(n)}$ can successively be determined from Eq. (6) whereas the low-energy parts $\mathbf{P}_\lambda X_\lambda^{(n)}$ can still be chosen arbitrarily. In the following we use for convenience $\mathbf{P}_\lambda X_\lambda^{(1)} = \mathbf{P}_\lambda X_\lambda^{(2)} = 0$ so that for the effective Hamiltonian $\mathcal{H}_\lambda$ up to second order in $\mathcal{H}_1$ follows

$$\mathcal{H}_\lambda = \mathcal{H}_0 + \mathbf{P}_\lambda \mathcal{H}_1 - \frac{1}{2} \mathbf{P}_\lambda \left[(\mathbf{Q}_\lambda \mathcal{H}_1), \frac{1}{\mathbf{L}_0} (\mathbf{Q}_\lambda \mathcal{H}_1) \right] - \mathbf{P}_\lambda \left[(\mathbf{P}_\lambda \mathcal{H}_1), \frac{1}{\mathbf{L}_0} (\mathbf{Q}_\lambda \mathcal{H}_1) \right] \tag{9}$$

Here ε was set equal to 1. The quantity $\mathbf{L}_0$ in (9) denotes the Liouville operator of the unperturbed Hamiltonian. It is defined by $\mathbf{L}_0 = [\mathcal{H}_0, A]$ for any operator A. Note that the perturbation expansion (9) can easily be extended to higher orders in ε. One should also note that the correct size dependence of the Hamiltonian is automatically guaranteed due to the commutators appearing in (9).

Next, let us use this perturbation theory to establish a renormalization approach by successively reducing the cutoff energy λ. In particular, instead of eliminating high-energy excitations in one step a sequence of stepwise transformations is used. Thereby, we obtain an effective model which becomes diagonal in the limit $\lambda \to 0$. In an infinitesimal formulation, the method yields renormalization equations as function of the cutoff λ. To find these equations we start from the renormalized Hamiltonian

$$\mathcal{H}_\lambda = \mathcal{H}_{0,\lambda} + \mathcal{H}_{1,\lambda} \tag{10}$$

after all excitations with energy differences larger than λ have been eliminated. Now we perform an additional renormalization of $\mathcal{H}_\lambda$ by eliminating all excitations inside an energy shell between λ and a smaller energy cutoff $(\lambda - \Delta\lambda)$ where $\Delta\lambda > 0$. The new Hamiltonian is found by use of (9)

$$\begin{aligned} \mathcal{H}_{(\lambda-\Delta\lambda)} = \mathbf{P}_{(\lambda-\Delta\lambda)} \mathcal{H}_\lambda - \frac{1}{2} \mathbf{P}_{(\lambda-\Delta\lambda)} \left[(\mathbf{Q}_{(\lambda-\Delta\lambda)} \mathcal{H}_{1,\lambda}), \frac{1}{\mathbf{L}_{0,\lambda}} (\mathbf{Q}_{(\lambda-\Delta\lambda)} \mathcal{H}_{1,\lambda}) \right] + \\ - \mathbf{P}_{(\lambda-\Delta\lambda)} \left[(\mathbf{P}_{(\lambda-\Delta\lambda)} \mathcal{H}_{1,\lambda}), \frac{1}{\mathbf{L}_{0,\lambda}} (\mathbf{Q}_{(\lambda-\Delta\lambda)} \mathcal{H}_{1,\lambda}) \right]. \end{aligned} \tag{11}$$

Here, $\mathbf{L}_{0,\lambda}$ denotes the Liouville operator with respect to the unperturbed part $\mathcal{H}_{0,\lambda}$ of the λ dependent Hamiltonian $\mathcal{H}_\lambda$. Note that the flow equations derived from Eq. (11) will lead to an approximative renormalization of $\mathcal{H}_\lambda$ because only contributions up to second order in $\mathcal{H}_{1,\lambda}$ are included in Eq. (11). For a concrete evaluation of Eq. (11) it is useful to divide the second order term on the r.h.s into two parts: The first one connects eigenstates of $\mathcal{H}_{0,\lambda}$ with the same energy. This part commutes with $\mathcal{H}_{0,\lambda}$ and can therefore be considered as renormalization of the unperturbed Hamiltonian

$$\mathcal{H}_{0,(\lambda-\Delta\lambda)} - \mathcal{H}_{0,\lambda} = -\frac{1}{2}\,\mathbf{P}_0 \left[(\mathbf{Q}_{(\lambda-\Delta\lambda)}\mathcal{H}_{1,\lambda}), \frac{1}{\mathbf{L}_{0,\lambda}}(\mathbf{Q}_{(\lambda-\Delta\lambda)}\mathcal{H}_{1,\lambda}) \right]. \tag{12}$$

In contrast the second part connects eigenstates of $\mathcal{H}_{0,\lambda}$ with different energies and represents a renormalization of the interaction part of the Hamiltonian

$$\begin{aligned}\mathcal{H}_{1,(\lambda-\Delta\lambda)} - \mathbf{P}_{(\lambda-\Delta\lambda)}\mathcal{H}_{1,\lambda} = &-\mathbf{P}_{(\lambda-\Delta\lambda)} \left[(\mathbf{P}_{(\lambda-\Delta\lambda)}\mathcal{H}_{1,\lambda}), \frac{1}{\mathbf{L}_{0,\lambda}}(\mathbf{Q}_{(\lambda-\Delta\lambda)}\mathcal{H}_{1,\lambda}) \right] \\ &-\frac{1}{2}\left(\mathbf{P}_{(\lambda-\Delta\lambda)} - \mathbf{P}_0\right) \left[(\mathbf{Q}_{(\lambda-\Delta\lambda)}\mathcal{H}_{1,\lambda}), \frac{1}{\mathbf{L}_{0,\lambda}}(\mathbf{Q}_{(\lambda-\Delta\lambda)}\mathcal{H}_{1,\lambda}) \right].\end{aligned} \tag{13}$$

Note that for small $\Delta\lambda$ only the mixed term, i.e., the first part on the r.h.s. of Eq. (13), contributes to the renormalization of $\mathcal{H}_{1,\lambda}$

$$\mathcal{H}_{1,(\lambda-\Delta\lambda)} - \mathbf{P}_{(\lambda-\Delta\lambda)}\mathcal{H}_{1,\lambda} \approx -\mathbf{P}_{(\lambda-\Delta\lambda)} \left[(\mathbf{P}_{(\lambda-\Delta\lambda)}\mathcal{H}_{1,\lambda}), \frac{1}{\mathbf{L}_{0,\lambda}}(\mathbf{Q}_{(\lambda-\Delta\lambda)}\mathcal{H}_{1,\lambda}) \right]. \tag{14}$$

In the limit $\Delta\lambda \to 0$, i.e. for vanishing shell width, equations (12) and (14) lead to differential equations for the Hamiltonian as function of the cutoff energy λ. The resulting equations for the parameters of the Hamiltonian are called flow equations. Their solution depend on the initial values of the parameters of the Hamiltonian. Note that for $\lambda \to 0$ the resulting Hamiltonian only consists of the unperturbed part $\mathcal{H}_{(\lambda\to 0)}$ so that an effectively diagonal Hamiltonian is obtained.

III. APPLICATION TO THE ELECTRON-PHONON SYSTEM

In this section we apply the renormalization approach discussed above to the system (1) of interacting electrons and phonons. The aim is to decouple the electron and the phonon subsystems. The Hamiltonian (1) is gauge invariant. In contrast, a BCS-like Hamiltonian breaks this symmetry. Thus, in order to describe the superconducting state of the system, the renormalized Hamiltonian should contain a symmetry breaking field. Therefore, our starting Hamiltonian $\mathcal{H}_\lambda$ reads

$$\mathcal{H}_\lambda = \mathcal{H}_{0,\lambda} + \mathcal{H}_{1,\lambda}, \tag{15}$$

after all excitations with energies larger than λ have been eliminated, where

$$\mathcal{H}_{0,\lambda} = \sum_{\mathbf{k},\sigma} \varepsilon_{\mathbf{k}}\, c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} + \sum_{\mathbf{q}} \omega_{\mathbf{q}}\, b^\dagger_{\mathbf{q}} b_{\mathbf{q}} - \sum_{\mathbf{k}} \left(\Delta_{\mathbf{k},\lambda}\, c^\dagger_{\mathbf{k},\uparrow} c^\dagger_{-\mathbf{k},\downarrow} + \Delta^*_{\mathbf{k},\lambda}\, c_{-\mathbf{k},\downarrow} c_{\mathbf{k},\uparrow} \right) + C_\lambda, \tag{16}$$

$$\mathcal{H}_{1,\lambda} = \mathbf{P}_\lambda \mathcal{H}_1 \;=\; \mathbf{P}_\lambda \sum_{\mathbf{k},\mathbf{q},\sigma} \left(g_{\mathbf{q}}\, c^\dagger_{\mathbf{k},\sigma} c_{(\mathbf{k}+\mathbf{q}),\sigma} b^\dagger_{\mathbf{q}} + g^*_{\mathbf{q}}\, c^\dagger_{(\mathbf{k}+\mathbf{q}),\sigma} c_{\mathbf{k},\sigma} b_{\mathbf{q}} \right). \tag{17}$$

The 'fields' $\Delta_{\mathbf{k},\lambda}$ and $\Delta^*_{\mathbf{k},\lambda}$ in $\mathcal{H}_{0,\lambda}$ couple to the operators $c^\dagger_{\mathbf{k},\uparrow} c^\dagger_{-\mathbf{k},\downarrow}$ and $c_{-\mathbf{k},\downarrow} c_{\mathbf{k},\uparrow}$ and break the gauge invariance. They will take over the role of the superconducting gap function but still depend on λ. The initial values for $\Delta_{\mathbf{k},\lambda}$ and the energy shift C_λ are those of the original model

$$\Delta_{\mathbf{k},(\lambda=\Lambda)} = 0, \quad C_{(\lambda=\Lambda)} \;=\; 0. \tag{18}$$

Note that renormalization contributions to the electron energies $\varepsilon_{\mathbf{k}}$, the phonon energies $\omega_{\mathbf{q}}$, and the electron-phonon interactions $g_{\mathbf{q}}$ have been neglected in (15). Also, additional interactions which would appear due to renormalization processes have been omitted. Let us first solve the eigenvalue problem of $\mathcal{H}_{0,\lambda}$. For this purpose, we perform a Bogoliubov transformation [11] and introduce new λ dependent fermionic quasi-particles

$$
\begin{aligned}
\alpha^\dagger_{\mathbf{k},\lambda} &= u^*_{\mathbf{k},\lambda} c^\dagger_{\mathbf{k},\uparrow} - v^*_{\mathbf{k},\lambda} c_{-\mathbf{k},\downarrow}, \\
\beta^\dagger_{\mathbf{k},\lambda} &= u^*_{\mathbf{k},\lambda} c^\dagger_{-\mathbf{k},\downarrow} + v^*_{\mathbf{k},\lambda} c_{\mathbf{k},\uparrow}
\end{aligned}
\tag{19}
$$

where

$$
\begin{aligned}
|u_{\mathbf{k},\lambda}|^2 &= \frac{1}{2}\left(1 + \frac{\varepsilon_{\mathbf{k}}}{\sqrt{\varepsilon^2_{\mathbf{k}} + |\Delta_{\mathbf{k},\lambda}|^2}}\right), \\
|v_{\mathbf{k},\lambda}|^2 &= \frac{1}{2}\left(1 - \frac{\varepsilon_{\mathbf{k}}}{\sqrt{\varepsilon^2_{\mathbf{k}} + |\Delta_{\mathbf{k},\lambda}|^2}}\right).
\end{aligned}
\tag{20}
$$

$\mathcal{H}_{0,\lambda}$ can be rewritten as

$$
\mathcal{H}_{0,\lambda} = \sum_{\mathbf{k}} E_{\mathbf{k},\lambda}\left(\alpha^\dagger_{\mathbf{k},\lambda}\alpha_{\mathbf{k},\lambda} + \beta^\dagger_{\mathbf{k},\lambda}\beta_{\mathbf{k},\lambda}\right) + \sum_{\mathbf{k}} (\varepsilon_{\mathbf{k}} - E_{\mathbf{k},\lambda}) + \sum_{\mathbf{q}} \omega_{\mathbf{q}}\, b^\dagger_{\mathbf{q}} b_{\mathbf{q}} + C_\lambda
\tag{21}
$$

where the fermionic excitation energies are given by $E_{\mathbf{k},\lambda} = \sqrt{\varepsilon^2_{\mathbf{k}} + |\Delta_{\mathbf{k},\lambda}|^2}$.

Next let us eliminate all excitations within the energy shell between λ and $(\lambda - \Delta\lambda)$ by applying the renormalization scheme of section II. We are primarily interested in the renormalization of the gap function $\Delta_{\mathbf{k},\lambda}$. Note that for this case we have to consider the renormalization contribution given by (14)

$$
\delta\mathcal{H}_1(\lambda, \Delta\lambda) := \mathcal{H}_{1,(\lambda-\Delta\lambda)} - \mathbf{P}_{(\lambda-\Delta\lambda)}\mathcal{H}_{1,\lambda}.
\tag{22}
$$

The reason is that the renormalization (12) of $\mathcal{H}_{0,\lambda}$ only gives contributions which connects eigenstates of $\mathcal{H}_{0,\lambda}$ with the same energy. Thus, this part only changes the quasiparticle energies from $E_{\mathbf{k},\lambda}$ to $E_{\mathbf{k},(\lambda-\Delta\lambda)}$. In contrast, the renormalization (22) changes the relative weight of the operator terms in (16) and is exactly the renormalization needed to describe the flow of $\Delta_{\mathbf{k},\lambda}$ which will be discussed in the following.

There is no principle problem to evaluate the renormalization contributions (14). First, one expresses the creation and annihilation operators by the quasiparticle operators (19) and uses the relation $\mathbf{L}_{0,\lambda}\alpha^\dagger_{k,\lambda} = E_{\mathbf{k},\lambda}\alpha^\dagger_{\mathbf{k},\lambda}$ and an equivalent relation for $\beta^\dagger_{\mathbf{k},\lambda}$ to evaluate the denominator in Eq. (14). Then the quasi-particle operators (18) have to be transformed back to the original electron operators. The main reason for this procedure is the fact that the Bogoliubov transformation (19),(20) depends on the cutoff λ. Thereby, a lot of terms arise which contribute to the renormalization (14). For convenience, we evaluate the denominator in Eq. (14) by use of the assumption $\varepsilon^2_{\mathbf{k}} \gg |\Delta_{\mathbf{k},\lambda}|^2$. As it turns out, the resulting flow equations still contain sums over $\mathbf{k}$. Note that the approximation used is valid for most of the $\mathbf{k}$ dependent terms (except for those $\mathbf{k}$ values close to the Fermi momentum). Thus, it does not strongly affected the renormalization contributions. The two operator expressions contributing to the commutator in (14) are given in this approximation by

$$
\mathbf{P}_{(\lambda-\Delta\lambda)}\mathcal{H}_{1,\lambda} = \sum_{\mathbf{k},\mathbf{q},\sigma} \Theta\left[(\lambda - \Delta\lambda) - |\varepsilon_{\mathbf{k}} - \varepsilon_{(\mathbf{k}+\mathbf{q})} + \omega_{\mathbf{q}}|\right]\left\{g_{\mathbf{q}}\, c^\dagger_{\mathbf{k},\sigma} c_{(\mathbf{k}+\mathbf{q}),\sigma} b^\dagger_{\mathbf{q}} + \text{h.c.}\right\},
\tag{23}
$$

$$
\frac{1}{\mathbf{L}_{0,\lambda}}\mathbf{Q}_{(\lambda-\Delta\lambda)}\mathcal{H}_{1,\lambda} = \sum_{\mathbf{k},\mathbf{q},\sigma} \frac{\delta\Theta_{\mathbf{k},\mathbf{q}}(\lambda, \Delta\lambda)}{\varepsilon_{\mathbf{k}} - \varepsilon_{(\mathbf{k}+\mathbf{q})} + \omega_{\mathbf{q}}}\left\{g_{\mathbf{q}}\, c^\dagger_{\mathbf{k},\sigma} c_{(\mathbf{k}+\mathbf{q}),\sigma} b^\dagger_{\mathbf{q}} - \text{h.c.}\right\}
\tag{24}
$$

where

$$
\delta\Theta_{\mathbf{k},\mathbf{q}}(\lambda, \Delta\lambda) = \Theta\left[|\varepsilon_{\mathbf{k}} - \varepsilon_{(\mathbf{k}+\mathbf{q})} + \omega_{\mathbf{q}}| - (\lambda - \Delta\lambda)\right] - \Theta\left[|\varepsilon_{\mathbf{k}} - \varepsilon_{(\mathbf{k}+\mathbf{q})} + \omega_{\mathbf{q}}| - \lambda\right]
\tag{25}
$$

describes the restriction to excitations on the energy shell $\Delta\lambda$. We are not interested in the renormalization of the phonon modes. Therefore all contributions including phonon operators are neglected. By using (23) and (24) we then find from (14)

$$\delta\mathcal{H}_1(\lambda,\Delta\lambda) = -\mathbf{P}_{(\lambda-\Delta\lambda)} \sum_{\mathbf{k},\mathbf{k}',\mathbf{q},\sigma,\sigma'} \frac{|g_\mathbf{q}|^2\,\delta\Theta_{\mathbf{k},\mathbf{q}}(\lambda,\Delta\lambda)\Theta\left[(\lambda-\Delta\lambda)-\left|\varepsilon_{\mathbf{k}'}-\varepsilon_{(\mathbf{k}'+\mathbf{q})}+\omega_\mathbf{q}\right|\right]}{\varepsilon_\mathbf{k}-\varepsilon_{(\mathbf{k}+\mathbf{q})}+\omega_\mathbf{q}} \times$$

$$\times \left\{ c^\dagger_{(\mathbf{k}+\mathbf{q}),\sigma} c_{\mathbf{k},\sigma} c^\dagger_{\mathbf{k}',\sigma'} c_{(\mathbf{k}'+\mathbf{q}),\sigma'} + \mathrm{h.c}\right\}. \tag{26}$$

In the following we restrict ourselves to renormalization contributions which lead to the formation of Cooper pairs. Consequently, the conditions $\mathbf{k}' = -(\mathbf{k}+\mathbf{q})$ and $\sigma' = -\sigma$ have to be fulfilled so that

$$-\lim_{\Delta\lambda\to 0}\frac{\delta\mathcal{H}_1(\lambda,\Delta\lambda)}{\Delta\lambda} = \tag{27}$$

$$= \sum_{\mathbf{k},\mathbf{q},\sigma} \Theta\left[\lambda - 2\left|\varepsilon_\mathbf{k}-\varepsilon_{(\mathbf{k}+\mathbf{q})}\right|\right]\Theta\left[\lambda-\left|\varepsilon_{(\mathbf{k}+\mathbf{q})}-\varepsilon_\mathbf{k}+\omega_\mathbf{q}\right|\right]\delta\left(\left|\varepsilon_\mathbf{k}-\varepsilon_{(\mathbf{k}+\mathbf{q})}+\omega_\mathbf{q}\right|-\lambda\right)\times$$

$$\times\frac{|g_\mathbf{q}|^2}{\varepsilon_\mathbf{k}-\varepsilon_{(\mathbf{k}+\mathbf{q})}+\omega_\mathbf{q}}\left\{c^\dagger_{(\mathbf{k}+\mathbf{q}),\sigma}c^\dagger_{-(\mathbf{k}+\mathbf{q}),-\sigma}c_{-\mathbf{k},-\sigma}c_{\mathbf{k},\sigma}+\mathrm{h.c}\right\}$$

results from (26). Here, $\Theta\left[\lambda-2\left|\varepsilon_\mathbf{k}-\varepsilon_{(\mathbf{k}+\mathbf{q})}\right|\right]$ is due to the projector operator $\mathbf{P}_{(\lambda-\Delta\lambda)}$ in (26). Note that the differential expression on the l.h.s. of (27) is different from the differential $d\mathcal{H}_{1,\lambda}/d\lambda$. This follows from the definition of $\delta\mathcal{H}_1(\lambda,\Delta\lambda) = \mathcal{H}_{1,(\lambda-\Delta\lambda)} - \mathbf{P}_{(\lambda-\Delta\lambda)}\mathcal{H}_{1,\lambda}$ which differs from $\Delta\mathcal{H}_1(\lambda,\Delta\lambda) = \mathcal{H}_{1,(\lambda-\Delta\lambda)} - \mathcal{H}_{1,\lambda}$ due to the second term. Next we can simplify the Θ-functions in Eq. (27) by discussing $\varepsilon_\mathbf{k}\geq\varepsilon_{(\mathbf{k}+\mathbf{q})}$ and $\varepsilon_{(\mathbf{k}+\mathbf{q})}>\varepsilon_\mathbf{k}$ separately. There are no contributions from the latter case. For $\varepsilon_\mathbf{k}\geq\varepsilon_{(\mathbf{k}+\mathbf{q})}$ the contribution from the first term in the curly bracket in (27) and from its conjugate can be combined. By exploiting the Θ-functions the result can be rewritten as

$$-\lim_{\Delta\lambda\to 0}\frac{\delta\mathcal{H}_1(\lambda,\Delta\lambda)}{\Delta\lambda} = \sum_{\mathbf{k},\mathbf{q},\sigma}\delta\left(\left|\varepsilon_\mathbf{k}-\varepsilon_{(\mathbf{k}+\mathbf{q})}\right|+\omega_\mathbf{q}-\lambda\right)\frac{|g_\mathbf{q}|^2\,\Theta\left[\omega_\mathbf{q}-\left|\varepsilon_\mathbf{k}-\varepsilon_{(\mathbf{k}+\mathbf{q})}\right|\right]}{\left|\varepsilon_\mathbf{k}-\varepsilon_{(\mathbf{k}+\mathbf{q})}\right|+\omega_\mathbf{q}}\times$$

$$\times c^\dagger_{(\mathbf{k}+\mathbf{q}),\sigma}c^\dagger_{-(\mathbf{k}+\mathbf{q}),-\sigma}c_{-\mathbf{k},-\sigma}c_{\mathbf{k},\sigma}. \tag{28}$$

Here, we have assumed $g_\mathbf{q}=g_{-\mathbf{q}}$. Eq. (28) describes the renormalization of the λ dependent Hamiltonian $\mathcal{H}_\lambda$ with respect to the cutoff λ. Next we use (28) to derive flow equations for the parameters $\Delta_{\mathbf{k},\lambda}$ and C_λ. For this purpose, a factorization with respect to the full Hamiltonian $\mathcal{H}$ is carried out. The final flow equations read

$$\frac{d\Delta_{\mathbf{k},\lambda}}{d\lambda} = -2\sum_\mathbf{q}\delta\left(\left|\varepsilon_\mathbf{k}-\varepsilon_{(\mathbf{k}+\mathbf{q})}\right|+\omega_\mathbf{q}-\lambda\right)\frac{|g_\mathbf{q}|^2\,\Theta\left[\omega_\mathbf{q}-\left|\varepsilon_\mathbf{k}-\varepsilon_{(\mathbf{k}+\mathbf{q})}\right|\right]}{\left|\varepsilon_\mathbf{k}-\varepsilon_{(\mathbf{k}+\mathbf{q})}\right|+\omega_\mathbf{q}}\left\langle c_{-(\mathbf{k}+\mathbf{q}),\downarrow}c_{(\mathbf{k}+\mathbf{q}),\uparrow}\right\rangle, \tag{29}$$

$$\frac{dC_\lambda}{d\lambda} = \sum_\mathbf{k}\left\langle c^\dagger_{\mathbf{k},\uparrow}c^\dagger_{-\mathbf{k},\downarrow}\right\rangle\frac{d\Delta_{\mathbf{k},\lambda}}{d\lambda}. \tag{30}$$

Note that in contrast to (28), Eqs. (29) and (30) are differential equations with normal derivatives of $\Delta_{\mathbf{k},\lambda}$ and C_λ. This fact can be explained as follows: As discussed above, the difference between the expressions $\delta\mathcal{H}_1(\lambda,\Delta\lambda) = \mathcal{H}_{1,(\lambda-\Delta\lambda)} - \mathbf{P}_{(\lambda-\Delta\lambda)}\mathcal{H}_{1,\lambda}$ and $\Delta\mathcal{H}_1(\lambda,\Delta\lambda)=\mathcal{H}_{1,(\lambda-\Delta\lambda)}-\mathcal{H}_{1,\lambda}$ is given by the quantity $\mathbf{Q}_{(\lambda-\Delta\lambda)}\mathcal{H}_{1,\lambda}$ which consists of all matrix elements of $\mathcal{H}_{1,\lambda}$ between eigenstates of $\mathcal{H}_{0,\lambda}$ with energy differences between $(\lambda-\Delta\lambda)$ and λ. We are interested in the new Hamiltonian $\mathcal{H}_{(\lambda-\Delta\lambda)} = \mathbf{P}_{(\lambda-\Delta\lambda)}\mathcal{H}_{(\lambda-\Delta\lambda)}$ which only contains transition operators between states with energy differences smaller than $(\lambda-\Delta\lambda)$. Therefore, all renormalization contributions which lead to matrix elements with energy differences larger than $(\lambda-\Delta\lambda)$ are not relevant. Thus, we obtain differential equations for the parameters of $\mathcal{H}_{(\lambda-\Delta\lambda)}$.

Note that the factor 2 in front of (29) is due to the sum over σ in (28). The expectation values $\langle\ldots\rangle$ in (29) and (30) are formed with the full Hamiltonian $\mathcal{H}$ and are independent of λ. The flow equations can be easily integrated between the lower cutoff ($\lambda\to 0$) and the cutoff Λ of the original model. The result is

$$\tilde\Delta_\mathbf{k} = \Delta_{\mathbf{k},\Lambda} + 2\sum_\mathbf{q}\frac{|g_\mathbf{q}|^2\,\Theta\left[\omega_\mathbf{q}-\left|\varepsilon_\mathbf{k}-\varepsilon_{(\mathbf{k}+\mathbf{q})}\right|\right]}{\left|\varepsilon_\mathbf{k}-\varepsilon_{(\mathbf{k}+\mathbf{q})}\right|+\omega_\mathbf{q}}\left\langle c_{-(\mathbf{k}+\mathbf{q}),\downarrow}c_{(\mathbf{k}+\mathbf{q}),\uparrow}\right\rangle, \tag{31}$$

$$\tilde C = C_\Lambda + \sum_\mathbf{k}\left\langle c^\dagger_{\mathbf{k},\uparrow}c^\dagger_{-\mathbf{k},\downarrow}\right\rangle\left(\tilde\Delta_\mathbf{k}-\Delta_{\mathbf{k},\Lambda}\right) \tag{32}$$

where a short hand notation for the desired values of $\Delta_{\mathbf{k},\lambda}$ and $C_{\mathbf{k},\lambda}$ at $\lambda = 0$ was introduced: $\tilde{\Delta}_{\mathbf{k}} = \Delta_{\mathbf{k},(\lambda\to 0)}$, $\tilde{C} = C_{(\lambda\to 0)}$. Note that $\tilde{\Delta}_{\mathbf{k}}$ and $\tilde{C}$ only depend on the parameters of the original system (1) and on $\Delta_{\mathbf{k},\Lambda}$ and C_Λ. The initial conditions (18) for $\Delta_{\mathbf{k},\Lambda}$ and C_Λ will be used later. For $\lambda \to 0$ the renormalized Hamiltonian $\tilde{\mathcal{H}} = \mathcal{H}_{(\lambda\to 0)}$ reads

$$\tilde{\mathcal{H}} = \sum_{\mathbf{k},\sigma} \varepsilon_{\mathbf{k}}\, c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} + \sum_{\mathbf{q}} \omega_{\mathbf{q}}\, b^\dagger_{\mathbf{q}} b_{\mathbf{q}} - \sum_{\mathbf{k}} \left(\tilde{\Delta}_{\mathbf{k}}\, c^\dagger_{\mathbf{k},\uparrow} c^\dagger_{-\mathbf{k},\downarrow} + \tilde{\Delta}^*_{\mathbf{k}}\, c_{-\mathbf{k},\downarrow} c_{\mathbf{k},\uparrow} \right) + \tilde{C}. \tag{33}$$

$\tilde{\mathcal{H}}$ can easily be diagonalized by a Bogoliubov transformation according to (19) and (20)

$$\tilde{\mathcal{H}} = \sum_{\mathbf{k}} \tilde{E}_{\mathbf{k}} \left(\tilde{\alpha}^\dagger_{\mathbf{k}} \tilde{\alpha}_{\mathbf{k}} + \tilde{\beta}^\dagger_{\mathbf{k}} \tilde{\beta}_{\mathbf{k}} \right) + \sum_{\mathbf{k}} \left(\varepsilon_{\mathbf{k}} - \tilde{E}_{\mathbf{k}} \right) + \sum_{\mathbf{q}} \omega_{\mathbf{q}}\, b^\dagger_{\mathbf{q}} b_{\mathbf{q}} + \tilde{C} \tag{34}$$

where $\tilde{E}_{\mathbf{k}} = E_{\mathbf{k},(\lambda\to 0)}$, $\tilde{\alpha}_{\mathbf{k}} = \alpha_{\mathbf{k},(\lambda\to 0)}$, and $\tilde{\beta}_{\mathbf{k}} = \beta_{\mathbf{k},(\lambda\to 0)}$.

Finally, we have to determine the expectation values in (31) and (32). Since $\tilde{\mathcal{H}}$ emerged from the original model $\mathcal{H}$ by an unitary transformation, the free energy can be calculated either from $\mathcal{H}$ or from $\tilde{\mathcal{H}}$

$$\begin{aligned} F &= -\frac{1}{\beta} \ln \operatorname{Tr} e^{-\beta \mathcal{H}} \; = \; -\frac{1}{\beta} \ln \operatorname{Tr} e^{-\beta \tilde{\mathcal{H}}}, \\ &= -\frac{2}{\beta} \sum_{\mathbf{k}'} \ln \left(1 + e^{-\beta \tilde{E}_{\mathbf{k}'}} \right) + \frac{1}{\beta} \sum_{\mathbf{q}} \left(1 - e^{-\beta \omega_{\mathbf{q}}} \right) + \sum_{\mathbf{k}'} \left(\varepsilon_{\mathbf{k}'} - \tilde{E}_{\mathbf{k}'} \right) + \tilde{C} \end{aligned} \tag{35}$$

where (34) was used. The required expectation values are found by functional derivative

$$\begin{aligned} \left\langle c^\dagger_{\mathbf{k},\uparrow} c^\dagger_{-\mathbf{k},\downarrow} \right\rangle &= -\frac{\partial F}{\partial \Delta_{\mathbf{k},\Lambda}} \\ &= \sum_{\mathbf{k}'} \frac{1 - 2f(\tilde{E}_{\mathbf{k}'})}{2\sqrt{\varepsilon^2_{\mathbf{k}'} + \left|\tilde{\Delta}_{\mathbf{k}'}\right|^2}} \left[\tilde{\Delta}^*_{\mathbf{k}'} \frac{\partial \tilde{\Delta}_{\mathbf{k}'}}{\partial \Delta_{\mathbf{k},\Lambda}} + \tilde{\Delta}_{\mathbf{k}'} \frac{\partial \tilde{\Delta}^*_{\mathbf{k}'}}{\partial \Delta_{\mathbf{k},\Lambda}} \right] + \frac{\partial \tilde{C}}{\partial \Delta_{\mathbf{k},\Lambda}} \\ &= \frac{\tilde{\Delta}^*_{\mathbf{k}} \left[1 - 2f(\tilde{E}_{\mathbf{k}}) \right]}{2\sqrt{\varepsilon^2_{\mathbf{k}} + \left|\tilde{\Delta}_{\mathbf{k}}\right|^2}} + \mathcal{O}\left(\left[\frac{|g_{\mathbf{q}}|^2}{\left|\varepsilon_{\mathbf{k}} - \varepsilon_{(\mathbf{k}+\mathbf{q})}\right| + \omega_{\mathbf{q}}} \right]^2 \right). \end{aligned} \tag{36}$$

Here, $f(\tilde{E}_{\mathbf{k}})$ denotes the Fermi function with respect to the energy $\tilde{E}_{\mathbf{k}}$. If we neglect higher order corrections, Eqs. (31) and (32) can be rewritten as

$$\tilde{\Delta}_{\mathbf{k}} = \sum_{\mathbf{q}} \left\{ \frac{2\,|g_{\mathbf{q}}|^2\, \Theta\left[\omega_{\mathbf{q}} - \left|\varepsilon_{\mathbf{k}} - \varepsilon_{(\mathbf{k}+\mathbf{q})}\right| \right]}{\left|\varepsilon_{\mathbf{k}} - \varepsilon_{(\mathbf{k}+\mathbf{q})}\right| + \omega_{\mathbf{q}}} \right\} \frac{\tilde{\Delta}^*_{\mathbf{k}+\mathbf{q}} \left[1 - 2f(\tilde{E}_{\mathbf{k}+\mathbf{q}}) \right]}{2\sqrt{\varepsilon^2_{\mathbf{k}+\mathbf{q}} + \left|\tilde{\Delta}_{\mathbf{k}+\mathbf{q}}\right|^2}}, \tag{37}$$

$$\tilde{C} = \sum_{\mathbf{k}} \left|\tilde{\Delta}_{\mathbf{k}}\right|^2 \frac{1 - 2f(\tilde{E}_{\mathbf{k}+\mathbf{q}})}{2\sqrt{\varepsilon^2_{\mathbf{k}+\mathbf{q}} + \left|\tilde{\Delta}_{\mathbf{k}+\mathbf{q}}\right|^2}} \tag{38}$$

where the initial conditions (18) were used. Note that Eq. (37) has the form of the usual BCS-gap equation. Thus, the term inside the brackets $\{\dots\}$ can be interpreted as the absolute value of the effective phonon-induced electron-electron interaction

$$V_{\mathbf{k},\mathbf{q}} = -\frac{2\,|g_{\mathbf{q}}|^2\, \Theta\left[\omega_{\mathbf{q}} - \left|\varepsilon_{\mathbf{k}} - \varepsilon_{(\mathbf{k}+\mathbf{q})}\right| \right]}{\left|\varepsilon_{\mathbf{k}} - \varepsilon_{(\mathbf{k}+\mathbf{q})}\right| + \omega_{\mathbf{q}}} \tag{39}$$

for the formation of Cooper pairs. In contrast to the usual BCS-theory, in the present formalism both the attractive electron-electron interaction (39) and the gap equation (37) were derived in one step by applying the renormalization procedure to the electron-phonon system (1).

Let us now compare the induced electron-elctron interaction (39) with Fröhlich's result [3]

$$V_{\mathbf{k},\mathbf{q}}^{\text{Fröhlich}} = \frac{2\,|g_{\mathbf{q}}|^2\,\omega_{\mathbf{q}}}{\left[\varepsilon_{\mathbf{k}} - \varepsilon_{(\mathbf{k}+\mathbf{q})}\right]^2 - \omega_{\mathbf{q}}^2}. \tag{40}$$

Note that (40) contains a divergency at $|\varepsilon_{\mathbf{k}} - \varepsilon_{(\mathbf{k}+\mathbf{q})}| = \omega_{\mathbf{q}}$. Furthermore, this interaction becomes repulsive for $\left|\varepsilon_{\mathbf{k}} - \varepsilon_{(\mathbf{k}+\mathbf{q})}\right| > \omega_{\mathbf{q}}$. Thus, a cutoff function $\Theta\left[\omega_{\mathbf{q}} - \left|\varepsilon_{\mathbf{k}} - \varepsilon_{(\mathbf{k}+\mathbf{q})}\right|\right]$ for the electron-electron interaction (40) is introduced by hand in the usual BCS-theory to suppress repulsive contributions to this interaction. In contrast our result (39) has no divergency and is always attractive. Furthermore, the cutoff function in Eq. (39) shows that the attractive interaction results from particle-hole excitations with energies $|\varepsilon_{\mathbf{k}} - \varepsilon_{(\mathbf{k}+\mathbf{q})}| < \omega_{\mathbf{q}}$. This result directly follows from the renormalization process.

Recently, Mielke [6] obtained a λ-dependent phonon-induced electron-electron interaction

$$V_{\mathbf{k},\mathbf{q},\lambda}^{\text{Mielke}} = -\frac{2\,|g_{\mathbf{q}}|^2}{\left|\varepsilon_{\mathbf{k}} - \varepsilon_{(\mathbf{k}+\mathbf{q})}\right| + \omega_{\mathbf{q}}}\ \Theta(|\varepsilon_{\mathbf{k}+\mathbf{q}} - \varepsilon_{\mathbf{k}}| + \omega_{\mathbf{q}} - \lambda) \tag{41}$$

where in (41) for convenience the λ-dependence of the electron and the phonon energies is suppressed. Apart from the λ-dependent Θ-function, the main difference to our result (39) is that the cutoff function $\Theta\left[\omega_{\mathbf{q}} - \left|\varepsilon_{\mathbf{k}} - \varepsilon_{(\mathbf{k}+\mathbf{q})}\right|\right]$ is not present in (41). This difference may result from Mielke's way of performing the similarity transformation [8,9] of the electron-phonon system (1). The similarity transformation is based on the introduction of continuous unitary transformations and is formulated in terms of differential equations for the parameters of the Hamiltonian. Like in our approach (see Sec. II) also the similarity transformation leads to a band-diagonal structure of the normalized Hamiltonian with respect to the eigen representation of the unperturbed Hamiltonian. Due to the renormalization processes also new couplings occur. Mielke has first evaluated the phonon-induced electron-electron interaction (41) by eliminating excitations with energies larger than λ. In particular, for an Einstein model with dispersion-less phonons of frequency ω_0 the interaction becomes independent of λ if λ is chosen less than ω_0. Of course, for this case and assuming $|\varepsilon_{\mathbf{k}+\mathbf{q}} - \varepsilon_{\mathbf{k}}| < \omega_{\mathbf{q}}$ Mielke's result (41) and the result (39) become the same. Keeping this interaction and neglecting at the same time the remaining part of the electron-phonon interaction with energies smaller than λ a BCS-like gap equation was derived by Mielke [6]. The main difference to our result (39) is the absence of the cutoff-function $\Theta\left[\omega_{\mathbf{q}} - \left|\varepsilon_{\mathbf{k}} - \varepsilon_{(\mathbf{k}+\mathbf{q})}\right|\right]$, which demonstrates that only particle-hole excitations with energies less than ω_q participate in the attractive interactions. However, note that by setting $\lambda = 0$ a finite value of the interaction remains in (41). This interaction is non-diagonal in the unperturbed Hamiltonian as used by Mielke, $\mathcal{H}_{0,\lambda}^{\text{Mielke}} = \sum_{\mathbf{k},\sigma} \varepsilon_{\mathbf{k},\lambda} c_{\mathbf{k},\sigma}^\dagger c_{\mathbf{k},\sigma} + \sum_{\mathbf{q}} \omega_{\mathbf{q}} b_{\mathbf{q}}^\dagger b_{\mathbf{q}}$. This seems to be a contradiction to the allowed properties for operators at $\lambda = 0$ which should commute with the unperturbed Hamiltonian.

Finally, by use of Wegner's flow equation method [7], Lenz and Wegner obtained the following phonon-induced electron-electron interaction

$$V_{\mathbf{k},\mathbf{q}}^{\text{Lenz/Wegner}} = -\frac{2\,|g_{\mathbf{q}}|^2\,\omega_{\mathbf{q}}}{\left[\varepsilon_{\mathbf{k}} - \varepsilon_{(\mathbf{k}+\mathbf{q})}\right]^2 + \omega_{\mathbf{q}}^2} \tag{42}$$

which is attractive for all $\mathbf{k}$ and $\mathbf{q}$ [5]. The result (42) is similar to (40) if $\omega_{\mathbf{q}} \geq \left|\varepsilon_{\mathbf{k}} - \varepsilon_{(\mathbf{k}+\mathbf{q})}\right|$ is fulfilled. In contrast to our result (39), the interaction (42) remains finite even for $\left|\varepsilon_{\mathbf{k}} - \varepsilon_{(\mathbf{k}+\mathbf{q})}\right| > \omega_{\mathbf{q}}$. Wegner's flow equation method [7] as well as the similarity transformation [8,9] are based on the introduction of continuous unitary transformations. Both methods are formulated in terms of differential equations for the parameters of the Hamiltonian. However, they differ in the generator of the continuous unitary transformation. This leads to the different results (41) and (42). A detailed comparison of the flow equation method and the similarity transformation can be found in Ref. [6].

IV. CONCLUSION

In this paper we have applied a recently developed renormalization approach [10] to the 'classical' problem of interacting electrons and phonons. By adding a small field to the Hamiltonian, which break the gauge symmetry, we directly derive a BCS-like gap equation for the coupled electron-phonon system. In particular, it is shown that the derived gap function results directly from the renormalization process. The effective phonon-induced electron-electron interaction is deduced from the gap equation. In contrast to the Fröhlich interaction [3] no singularities appear in the effective interaction. Furthermore, the cutoff function which is included in Fröhlich's result by hand to avoid

repulsive contributions to the electron-electron interaction follows directly from the renormalization procedure. This means that phonon-induced particle-hole excitations only contribute to the attractive electron-electron interaction if their energies are smaller than the energy of the exchanged phonon.

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